Radiation Absorption in Fuel Rich Cores of Methanol Pool Fires

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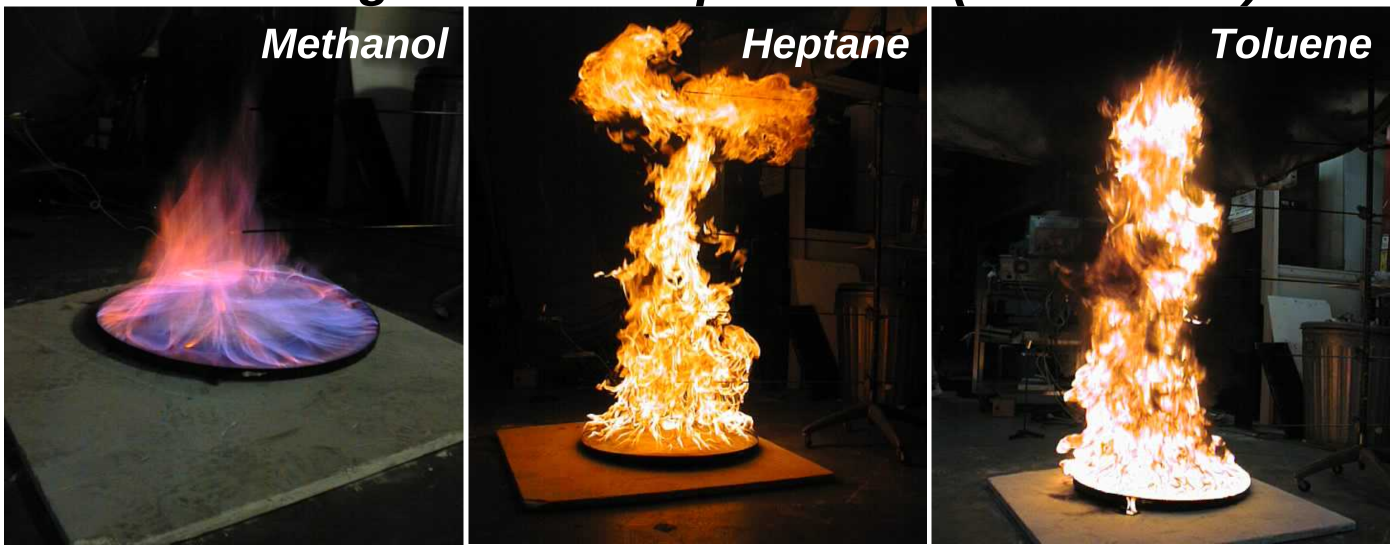
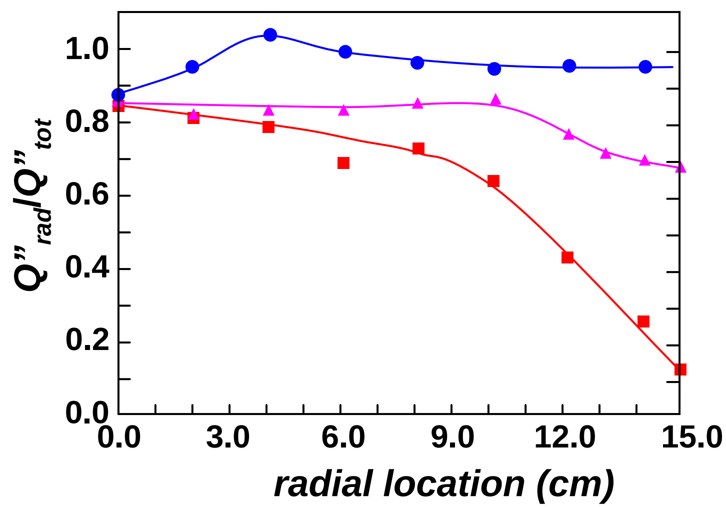
- **Program Manager at BFRL/NIST**
  - Dr. Jiann Yang

Radiation Feedback to Fuel Surface

Images of 45 cm pool fires (from BFRL)



Measurements of radiative feedback in 30 cm liquid pool fires Hamins et al. (1994)



Fraction of heat feedback to pool due to radiation

Toluene $Q_{rad}/Q_{tot} = 0.96$

Heptane $Q_{rad}/Q_{tot} = 0.80$

Methanol $Q_{rad}/Q_{tot} = 0.55$

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Objectives of the Program

- Develop methodology for building absorption coefficient (κ) database for species in fuel rich cores of fires
- Evaluate the impact of fuel absorption on radiative transport in liquid pool fires
- Integrate the database into Fire Dynamic Simulator for more effective radiative transport calculations
- Demonstrate the effectiveness of radiation database for extracting species profiles in fires

Absorption Coefficient Database

- **New database from current study expands RADCAL**
  - *Improved resolution as well as increased number of species*
- **Implements user-defined spectrally resolved tables with fits for finding absorption coefficients at any arbitrary temperature**

	HITEMP	RADCAL	New Database
Study	Rothman et al. (2003)	Grosshandler (1993)	This study
Temperature	≤ 1000 K	≤ 2000 K	≤ 1000 K with possible extrapolation
Species	3	5	12+
Combustion products	CO_2, H_2O, CO	CO_2, H_2O, CO, Soot	CO_2, H_2O, CO
Fuel	N/A	CH_4	CH_4, CH_3OH, C_2H_4, C_2H_6, C_3H_6, n-C_3H_8, $C_5H_8O_2$, n-C_7H_8, n-C_7H_{16}

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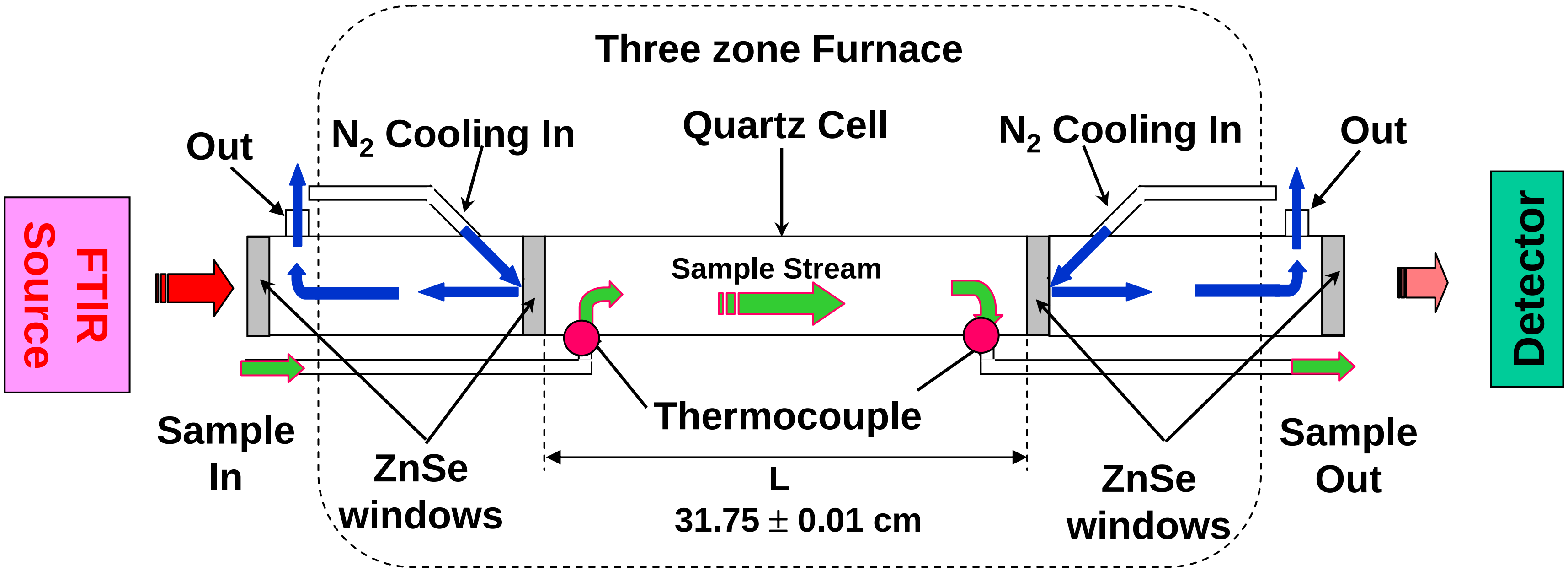
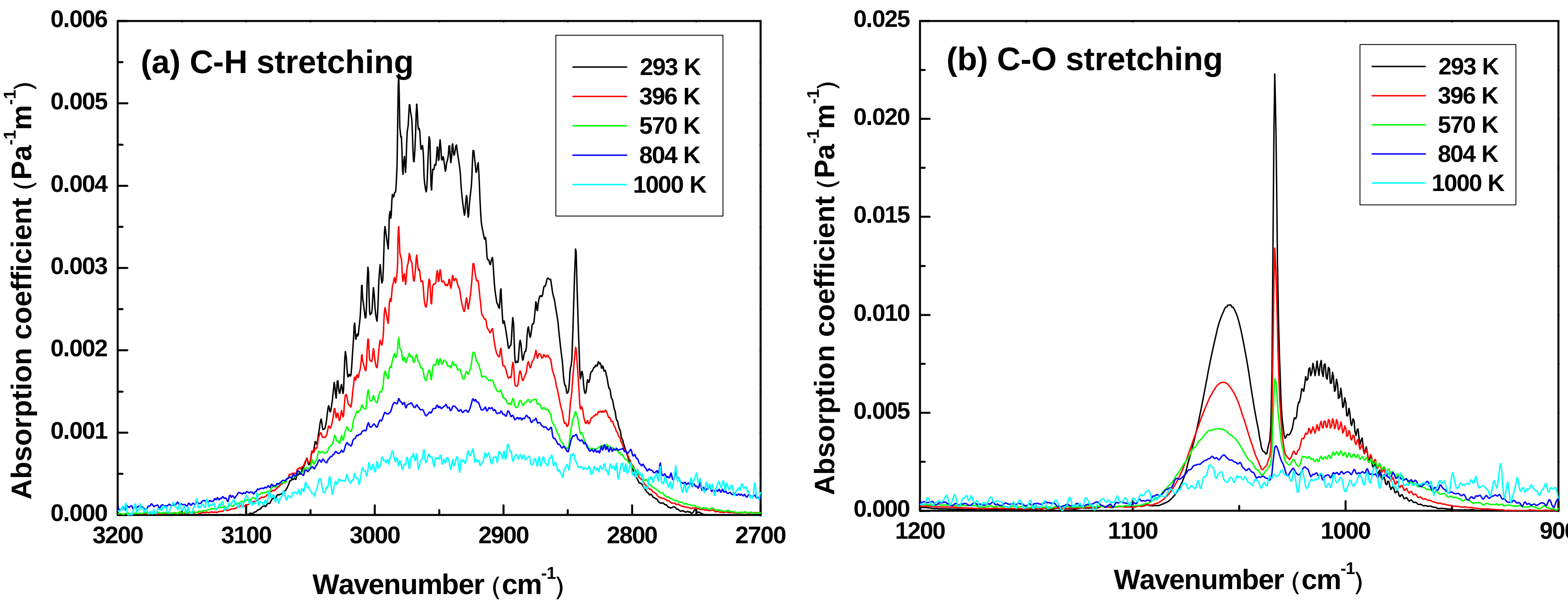
High Temperature FTIR Absorption Measurements



- Gaseous Species – n-C_3H_8, C_3H_6, C_2H_6 , C_2H_4, CH_4
- Liquid Fuels – n-C_7H_{16}, CH_3OH, C_7H_8, $C_5H_8O_2$
- Absorption measurements from 300 to 1000 K for 3 concentrations.

Absorption Coefficient Measurements for Methanol

- **Measured spectral absorption coefficients for CH_3OH for a range of temperatures. Bands are shown that provide significant radiative absorption: (a) C-H stretching band and (b) C-O stretching band.**



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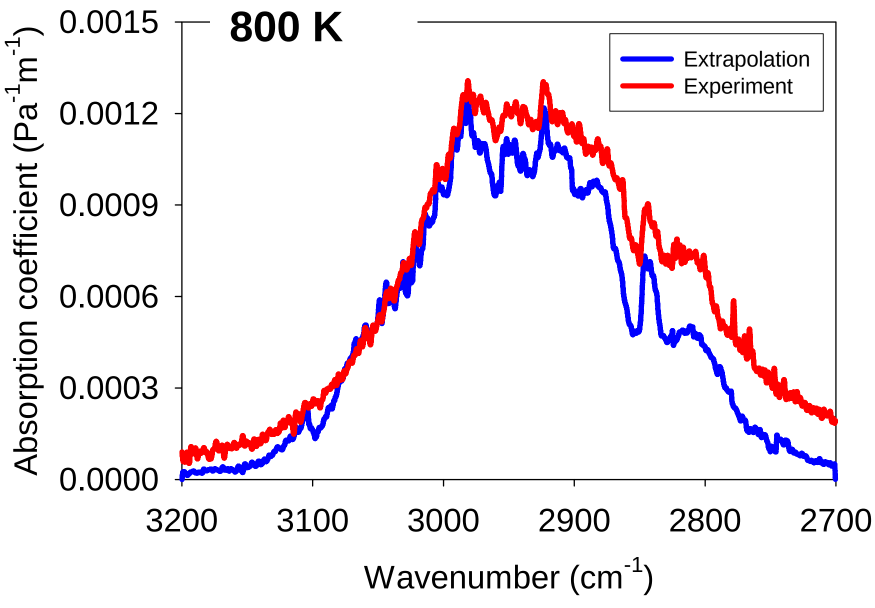
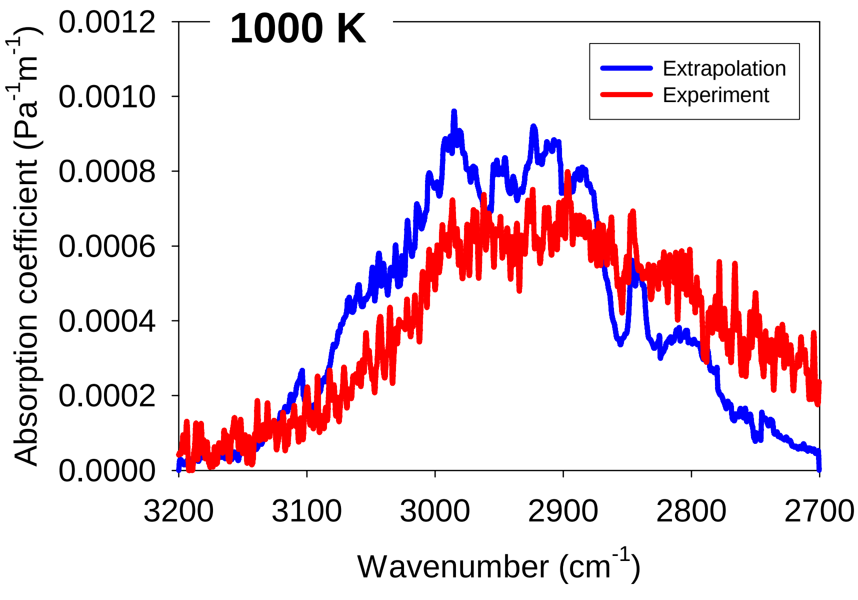
High Temperature Fits of Absorption Data for Interpolation with Methanol Data

Comparison of C_7H_8, CH_3OH, and n-C_7H_{16} data at 800 K with 1 cm^{-1} resolution to fits extrapolation from 300-600 K measurements

$$\kappa_\upsilon = \frac{S_0 \cdot \nu \cdot \left[1 - \exp\left(-\frac{1.439 \cdot \nu}{T}\right)\right] \cdot \exp\left(-\frac{1.439 \cdot \nu_r}{T}\right)}{T^n}$$

(developed by Fuss et al. 2001) with three fit parameters S_0, ν_r, and n

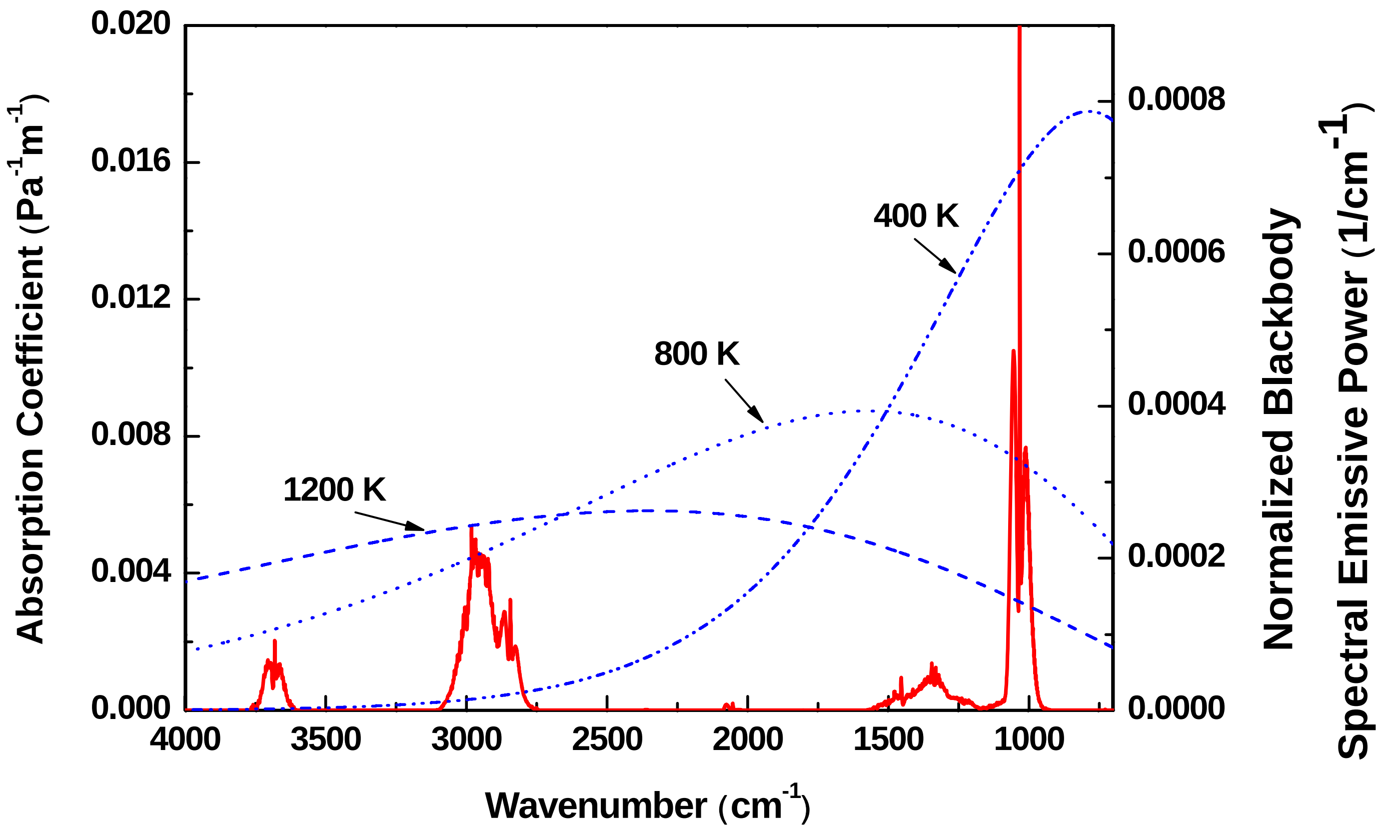




Integrated Error with 1.0 cm^{-1} resolution @ 800 K: –20.1% @ 1000 K: –5.1%

Planck Mean Absorption Coefficient for Methanol

- **Measured spectral absorption coefficient of methanol at 300 K and normalized blackbody spectral emissive power for various T.**

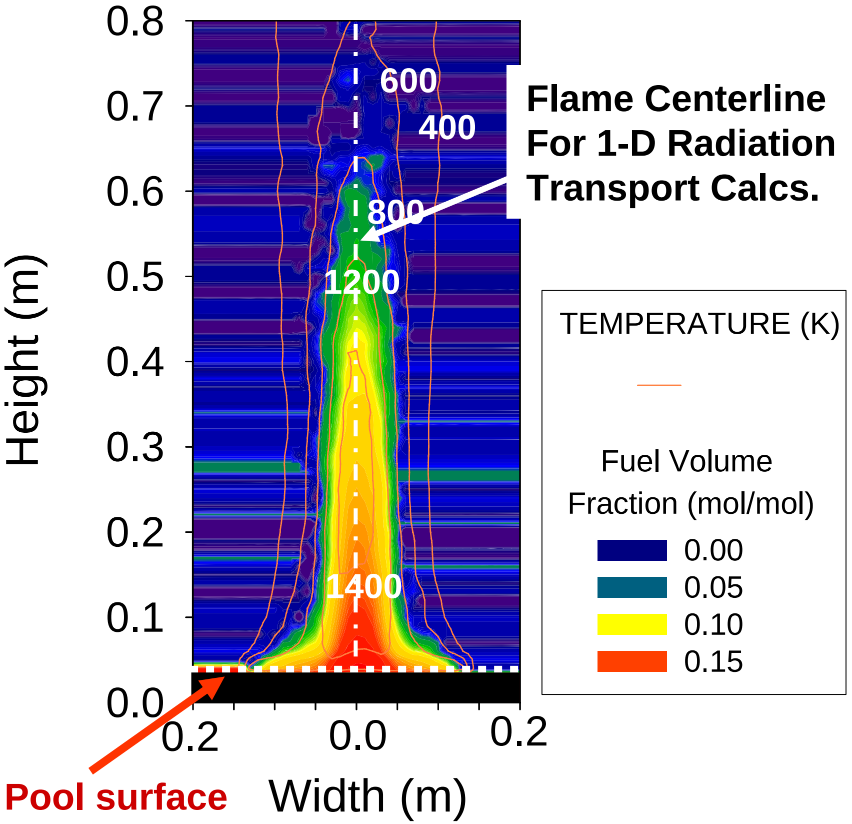


Use of FDS for Incident Thermal Radiation Feedback Analysis

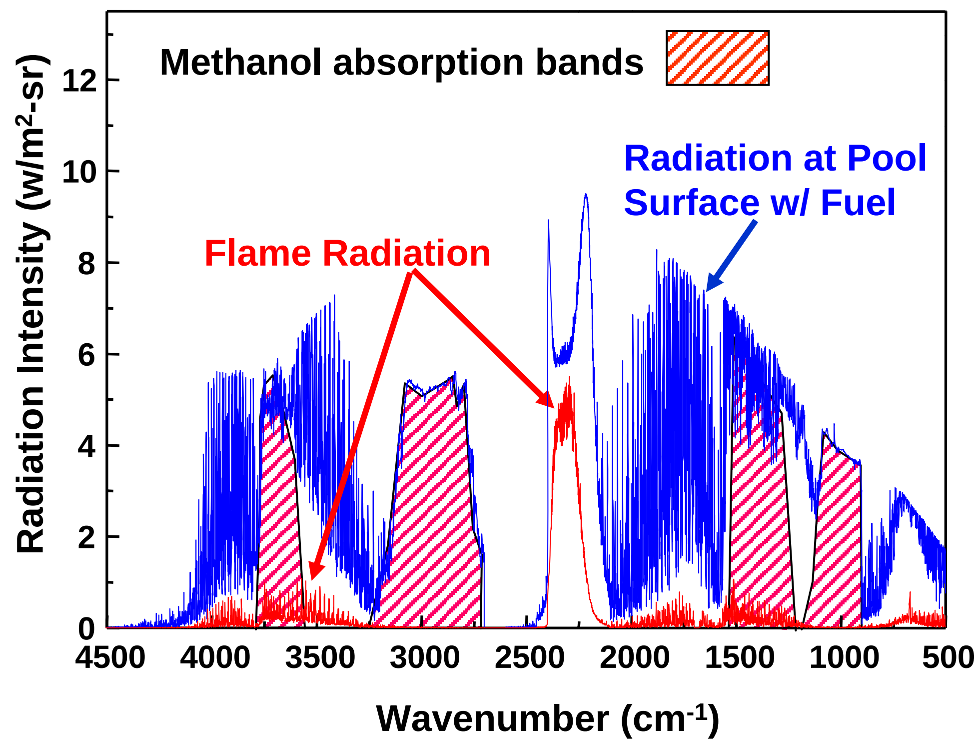
- **Use Fire Dynamic Simulator (FDS 4.02) to generate species and temperature profiles in 30 cm diameter pool fires**
  - profiles determined with 10 s of averaging in computational time after steady-state achieved in LES simulations
  - three fuels studied (CH_3OH as shown here, C_7H_{16}, C_7H_8)
- **Send FDS centerline results to Matlab-based code for doing 1-D centerline radiative transport calculations**
  - Use fuel specific temperature-dependent and independent absorption coefficients for spectrally-resolved radiation calculations
    - *FDS incorrectly assumes all fuels have CH_4 like absorption*
  - Use different flame boundary conditions for calculations
    - *Emission from species concentrations calculated by FDS at selected flame temperature – $I_{species}$*
    - *Plus blackbody emission at 1400 K for fuels with high degrees of sooting (heptane and toluene) – I_{BB}*

Calculated Energy Feedback to Methanol Pool Surface

Predicted Temperature/Fuel contour plot of 0.3 m methanol pool fire using NIST Fire Dynamics Simulator



1-D methanol pool radiation transport calculations along flame centerline with post-processing of FDS profiles



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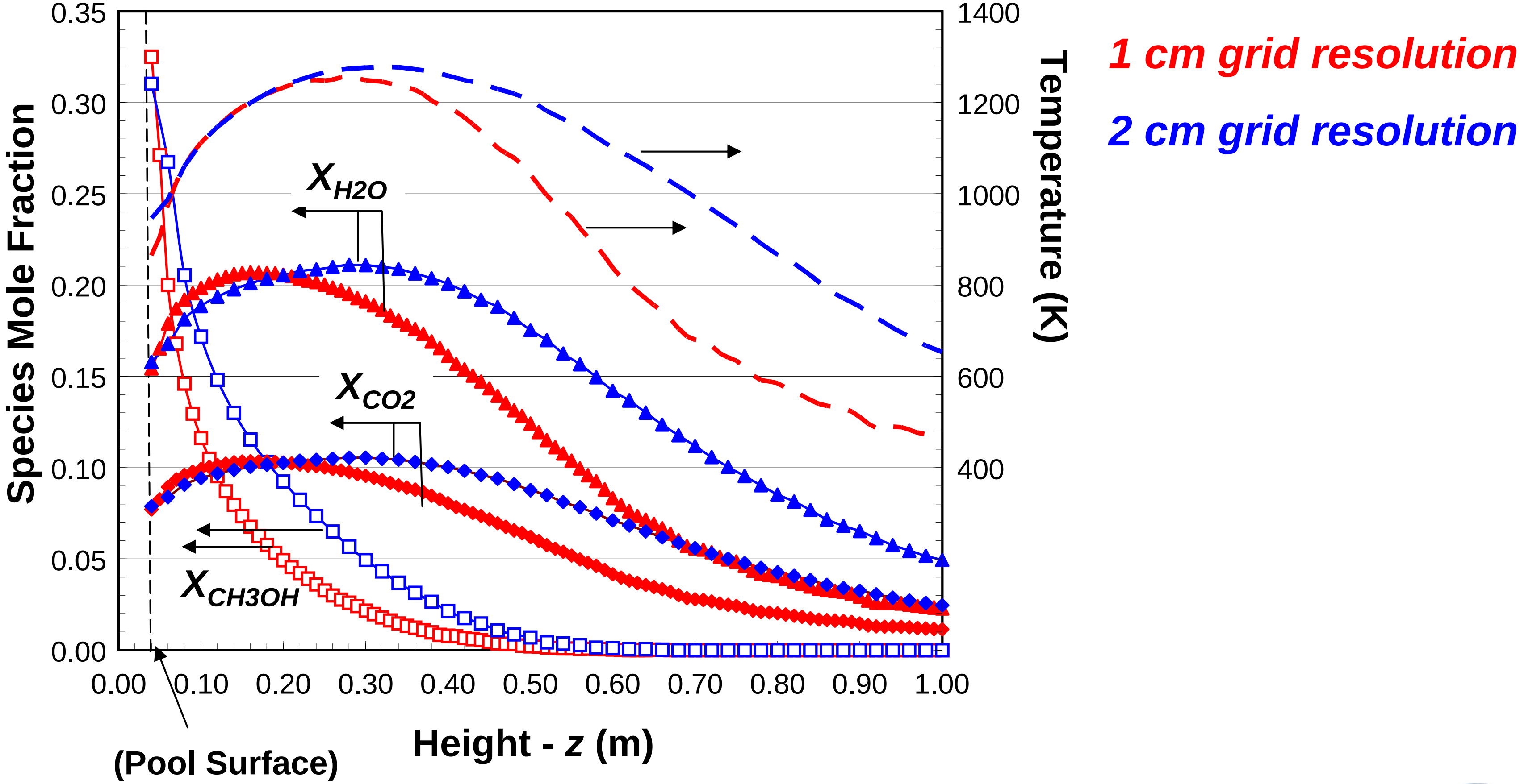
FDS Simulation for Methanol Pool Fire (d_{pool} = 0.3 m)

- **Temperature and major species mole fractions as a function of height for 0.3 m methanol pool fire by Fire Dynamic Simulator (v. 4.02).**
- **Results for 2 cm grid resolution show broader flame vs. 1 cm grid.**



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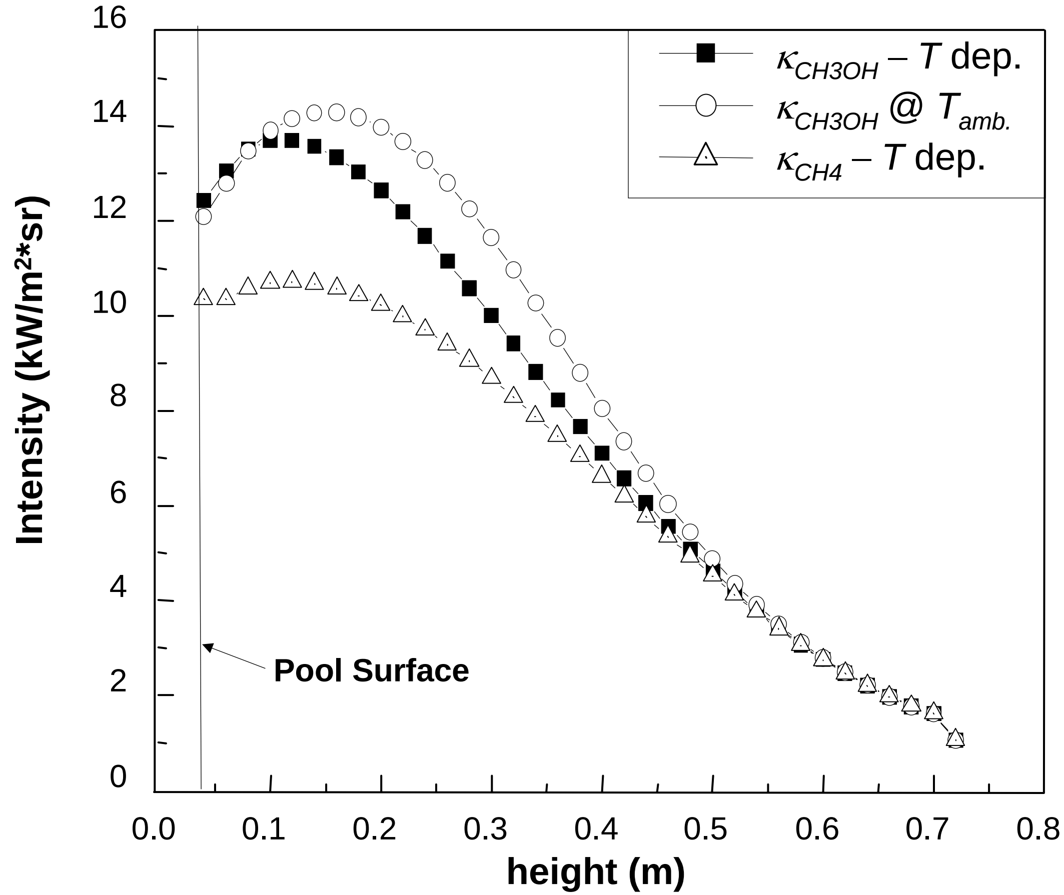
Radiation Calculations for Methanol Pool Fire

- **Integrated directional radiation intensity vs. height for different models of fuel absorption coefficient for 0.3 m methanol pool fire.**

- **Temperature-dependent κ_{CH3OH} gives outstanding agreement with experiments by Klassen et al. (1996)**
  - ***12.2 kW/m^2*sr for calcs.***
  - ***12.4 kW/m^2*sr for expts.***

- **Poor agreement between calculations and experiments with sooty pool fires of heptane and toluene**



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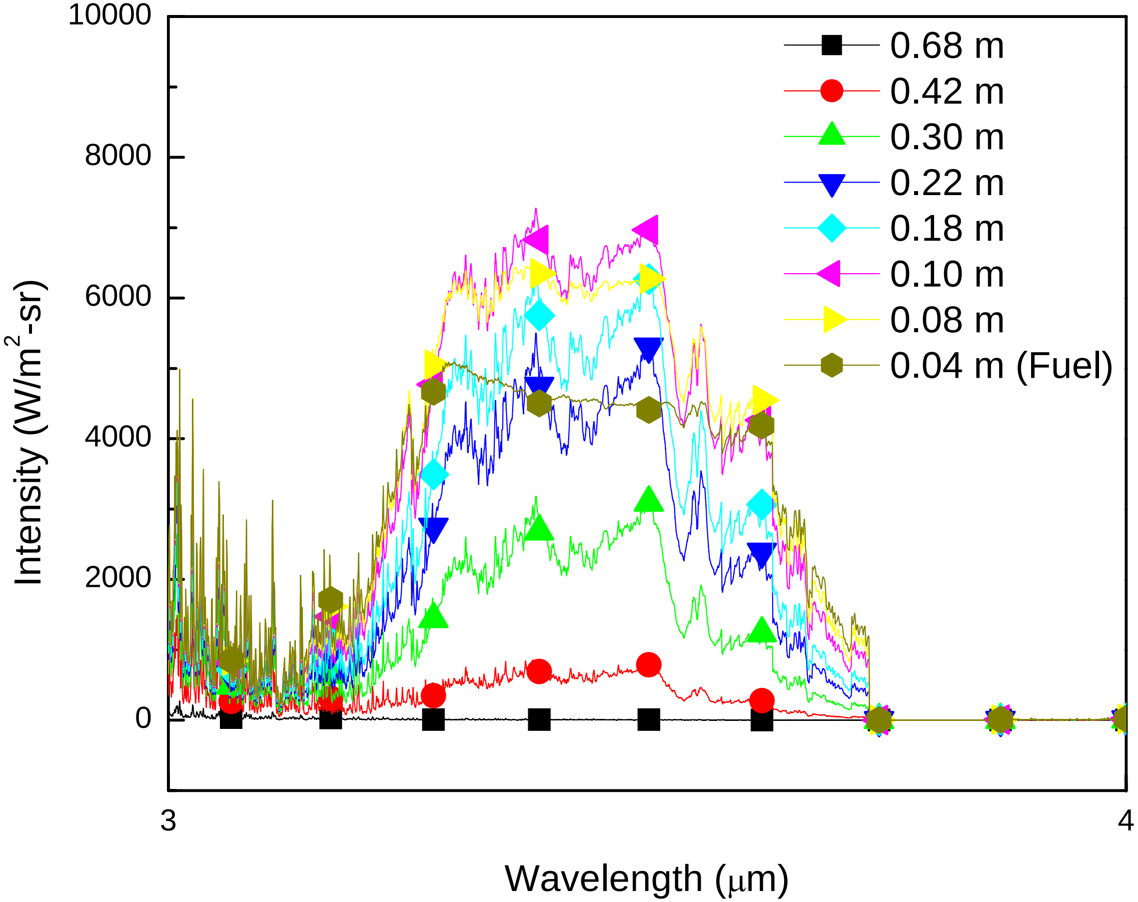
Challenge in Reconstructing Fuel Composition as a Function of Height with *IR* Measurements

- **Emissions or non-FTIR absorption data in flame are complicated by re-emission.**
- **Temperature-dependent absorption/emission results in non-monotonic signal strengths as a function of flame height**
- **This suggests the need for FTIR for monotonic transmissivity measurements**

Spectral radiation intensity of C-H stretching of CH_3OH about 3.4 mm (3000 cm^{-1}) as a function of height



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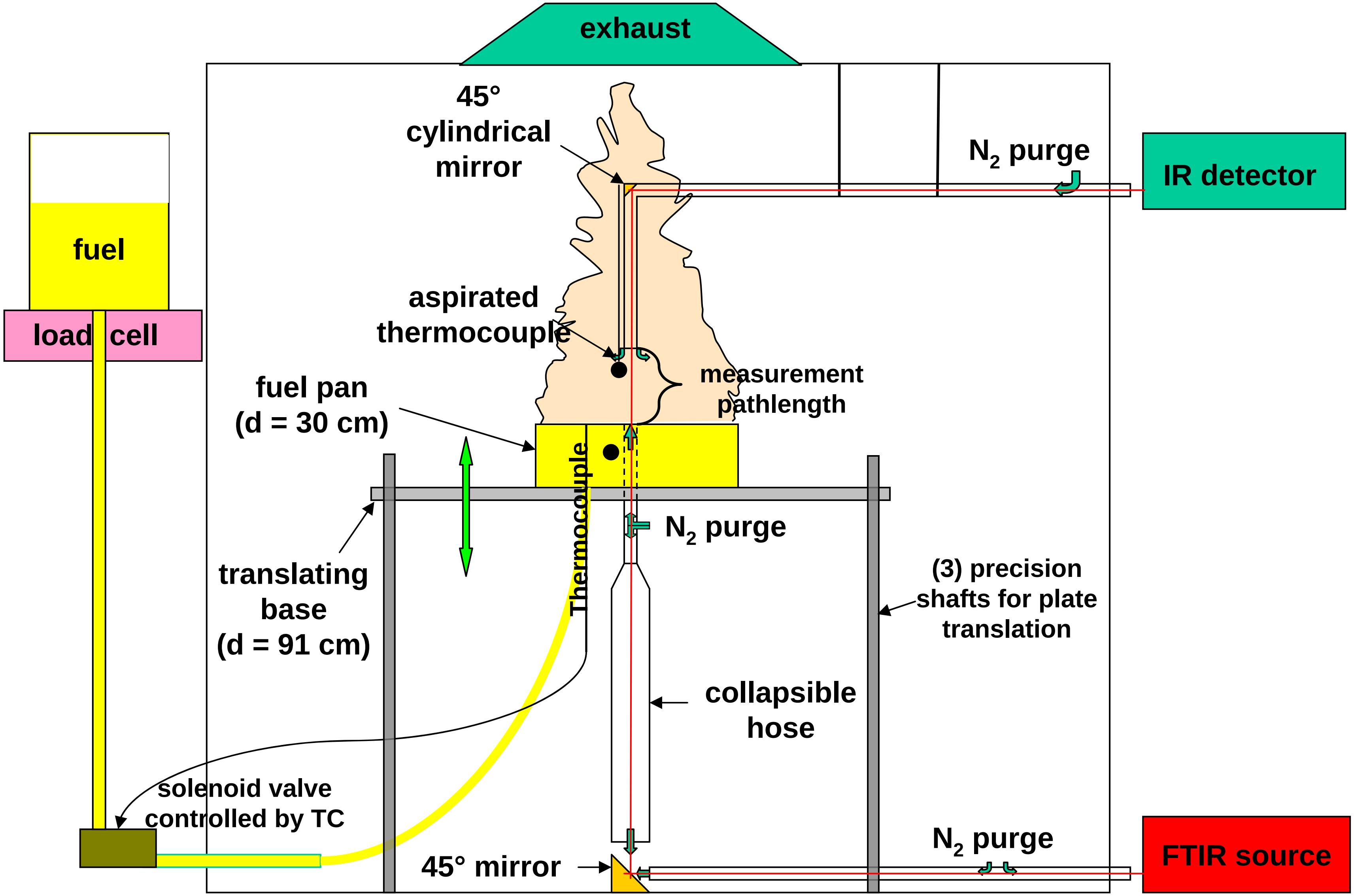
Experimental Measurements of Centerline Pool Fire Radiation (FTIR) Transmission

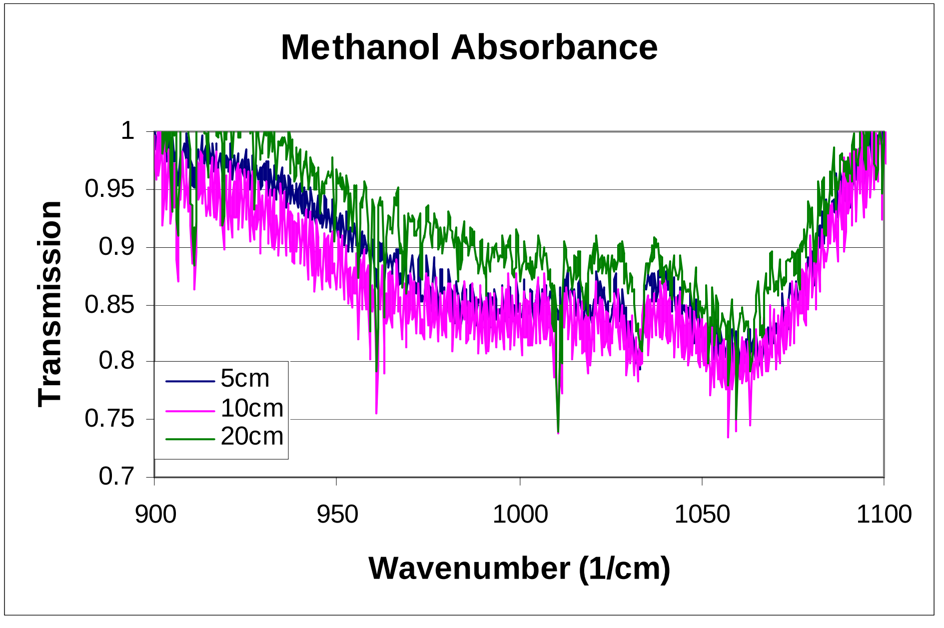
- **30 cm pool with centerline hole (N_2-purged) for FTIR signal up through fire**
- **Right angle probe (N_2-purged) for capturing transmitted radiation measurements**
  - Pathlength is set by adjusting the fuel pan height
  - Fuel pan and optical probe are water cooled
- **Burning rate measured by TC at pool surface to maintain constant liquid fuel depth (with load cell used for fuel supply rate)**
- ***Near centerline aspirated thermocouple readings for approximate T's***
- **Background FTIR spectrometer scan taken without fire**
  - *0.5 cm^{-1} resolution, with averaging over 128 scans*
- **Fire started, allowed to reach steady-state ~ 15 minutes**
- **FTIR spectrometer measures transmission along pathlength.**
  - *0.5 cm^{-1} resolution, 128 scan average*
  - *Samples divided by processed background spectrum to calculate transmission*
- **Pan height relative to probe adjusted for next measurements**

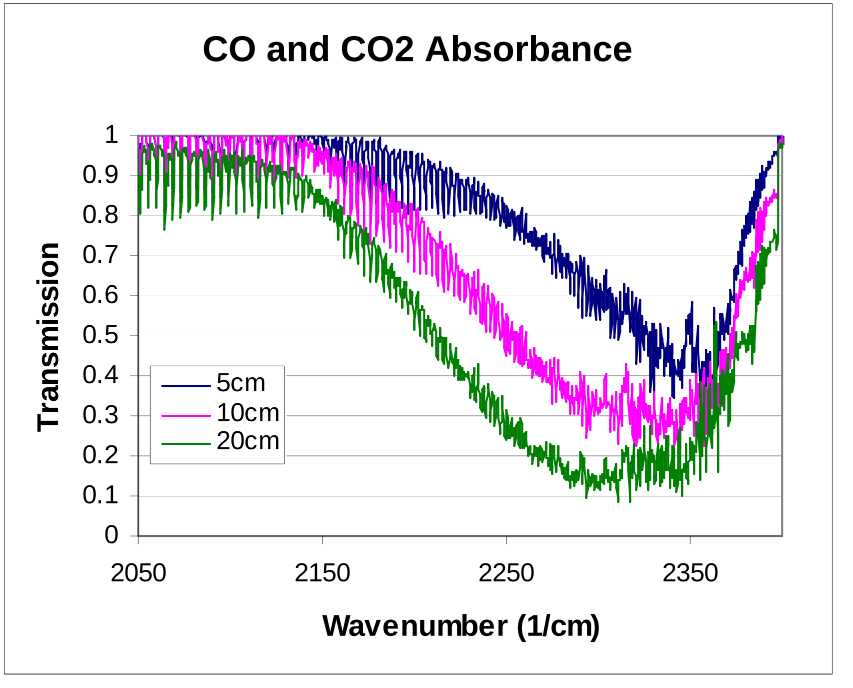
Pool Fire Radiation Measurements with *in situ* FTIR



Experimental Measurements of Centerline Pool Fire Radiation Transmission

- **Preliminary FTIR transmission measurements on 0.3 cm methanol pool taken at 5 and 10 cm intervals along pool fire centerline.**
- **FTIR optics in need of repair and did not permit high quality measurements for fitting absorption to species profiles.**
- **Repairs completed and further testing to be completed in April 2007.**





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Extracting Species Profiles from Transmission Measurements – Optimization Tool

- **Matlab-based function accesses high-temperature absorption coefficient database (0.48 cm^{-1} resolution) to calculate spectrally-resolved transmission over a path with given X_k and T profiles.**
- **Optimization (fmincon) is used to calculate differences compares calculated values for user-selected bands (or peaks) as a function of fitted X_k profiles to determine species profiles.**
  - *Optimization function*

$$F\left(\vec{X}_k\left(z_{meas}\right)\right)=\sum_{zmeas}\left(\sum_{waven}\left(\frac{\left(\tau_{calc,waven,zmeas}\left(\vec{X}_k\left(z_{meas}\right),\vec{T}\right)\right)}{\tau_{meas,waven,zmeas}}-1\right)^2\right)$$

  - *Model currently uses measured or FDS calculated T profile*
  - *Linear or spline fits between 5 cm measurements appears accurate enough to capture shape as indicated by FDS calculated profiles.*
- ***Calculations have been performed on preliminary measurements for X_{CH3OH} and X_{CO} but results give profiles < 50% of predicted FDS profiles.***
- ***Improved FDS optics to provide better measurements for code testing.***

Proposed Further Work (Spring and Summer 2007)

- **Take measurements *in situ* of IR transport through liquid pool fires along pool fire centerline.**
  - Fuels: methanol and heptane
  - Calculate centerline species profiles with Matlab-based optimization tool
- **Program the database and user expandibility into Fire Dynamics Simulator and explore how new radiation information affects incident heat flux on fuel surface and mass burning rates.**
- **Work with collaborators using new absorption coefficient database to perform improved fire calculations as well as data analysis**
  - Implement database in user-expandable RADCAL-like database